Amendment to the Claims:

This listing of claims will replace all prior versions, and listing, of claims in the application.

Listing of Claims:

1. (currently amended) A computer implemented method of ~~selecting a~~ generating representative three dimensional ~~conformation~~ conformations of reactant molecules comprising the steps of:

a) defining a set of topomeric alignment rules; and

b) applying the topomeric alignment rules to the reactants to generate the representative conformations.

2. (new) A computer implemented method of generating representative three dimensional conformations of fragments comprising the steps of:

a) defining a set of topomeric alignment rules; and

b) applying the topomeric alignment rules to the fragments to generate the representative conformations.

3. (new) A computer implemented method of characterizing the three dimensional structure of reactants, which can assume many conformations, comprising the steps of:

a) generating representative three dimensional conformations of reactant molecules comprising the steps of:

(1) defining a set of topomeric alignment rules; and

(2) applying the topomeric alignment rules to the reactants to generate the

representative conformations; and

b) determining the CoMFA steric fields for each aligned reactant.

4. (new) The method of claim 3 further comprising the addition of topomeric hydrogen bonding fields to the CoMFA steric fields.

5. (new) A computer implemented method of characterizing the three dimensional structure of fragments, which can assume many conformations, comprising the steps of:

a) generating representative three dimensional conformations of fragments comprising the steps of:

(1) defining a set of topomeric alignment rules; and

(2) applying the topomeric alignment rules to the fragments to generate the representative conformations; and

b) determining the CoMFA steric fields for each aligned fragment.

6. (new) The method of claim 5 further comprising the addition of topomeric hydrogen bonding fields to the CoMFA steric fields.

7. (new) A computer implemented method of applying a molecular structural descriptor to a set of reactants comprising the following steps:

a) generating representative three dimensional conformations of reactant molecules comprising the steps of:

(1) defining a set of topomeric alignment rules; and

(2) applying the topomeric alignment rules to the reactants to generate the representative conformations; and

b) determining the CoMFA steric fields for each topomerically aligned reactant; and

c) calculating the field differences between all pairs of reactants.

8. (new) The method of claim 7 further comprising after step b the additional step of adding topomeric hydrogen bonding fields to the CoMFA fields.

9. (new) A computer implemented method of applying a molecular structural descriptor to a set of fragments comprising the following steps:

a) generating representative three dimensional conformations of fragments comprising the steps of:

(1) defining a set of topomeric alignment rules; and

(2) applying the topomeric alignment rules to the fragments to generate the representative conformations; and

b) determining the CoMFA steric fields for each topomerically aligned fragment; and

c) calculating the field differences between all pairs of fragments.

10. (new) The method of claim 9 further comprising after step b the additional step of adding topomeric hydrogen bonding fields to the CoMFA fields.